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Two ways are given for solving the problem of the dependence of the refraction on the direction of magnetization on both sides of the refractive boundary, one applying the Halpern magnetic scattering vector, the other applying the dynamical theory of diffraction. They lead to different results. Experimental investigation of refraction by magnetic boundaries shows no dependence of the angle of deflection on the relative angles of magnetization in adjacent domains. This behaviour is only described correctly by the dynamical theory, which far from Laue reflections leads to a treatment by the Schrödinger equation with a spin-dependent potential dependent on the average continuous homogenous magnetic induction, both for the law of refraction and for the precession of the spin. The results of this treatment are discussed as a consequence of the behaviour of the spin of the neutrons. This gives some insight about how and why, with refraction, the intensities of the direct and deflected beams depend on the magnetization directions in adjacent domains. The dynamical theory also shows that the Halpern magnetic scattering vector applies only with Laue or Bragg reflections and not with transmission far from those reflections.

Introduction

This and the following paper (Schärpf, 1978 - paper II) present the fundamentals of magnetic scattering if it is not treated in the Born approximation. Scattering angle and intensity are treated with a specialized magnetic configuration, which can easily be realized in an experimental set up, i.e. Bloch walls. The first contribution treats the determination of the angle of deflection by magnetic refraction at domain boundaries i.e. the scattering angle; the second contribution treats the behaviour of neutrons in helical structures and its effect on the intensity of the neutron small-angle scattering by Bloch walls.

Bloch walls are plane parallel plates of thickness of the order of $10^3$ Å with the orientation of the magnetization changing continuously over this distance. The behaviour of the neutrons in this region is treated in the companion paper II, but from physical optics it is known that the deviation by refraction of the beam traversing a plane parallel plate is given by the two refractive indices of the adjacent media [see also equation (8) of paper II]. For the calculation of the angle of refraction it is therefore not necessary to investigate the behaviour in the interior of the walls themselves. One can consequently regard the Bloch wall as infinitely thin for the problem of the determination of the angle of deflection.

For Bloch walls of the geometry shown in Fig. 1 one has to establish the effect on neutrons of boundaries with one well-defined component of magnetization, normal to the boundary, being the same on both sides of the boundary and only one component ($B_z$) parallel to the boundary, changing its sign (Fig. 2). Such a configuration of magnetization only appears to be possible with Bloch walls, but is of fundamental interest, as one can see in the obviously fragmentary information which can be obtained from literature relative to this problem. There seems to be the solution in Bacon's (1975) book, where one can read that:

The problem of magnetic refraction at domain boundaries has been investigated fully by Hughes, Heller & Wallace (1949). The fundamental relation necessary in understanding this refraction is the refractive index

$$n^2 = 1 - \left[ \frac{N \lambda^2}{\pi} b \pm \mu_n \frac{B}{E} \right]. \quad (1)$$

$N = \text{atomic density}, \lambda = \text{neutron wavelength}, b = \text{coherent scattering length}, B = \text{magnetic induction}, \mu_n = \text{magnetic moment of the neutron}, E = \text{energy of the incident neutron}.$
Experimental measurements with magnetized mirrors have indeed decided in favor of the magnetic term as given in equation (1).

But with these mirrors the magnetization direction always lies in the plane of the refractive boundary. In our case there remains one component normal to the boundary on both sides of the boundary (Figs. 1 and 2) and the experiments of Hughes & Burgy (1951) do not bear upon this problem. In Bacon (1975) one also reads that: 'As a neutron proceeds through the iron from domain to domain it will undergo refraction at the intervening boundaries, suffering deviations which will depend on the orientation of the boundary and the directions of the magnetization on the two sides of it.'

Equation (1) does not include an indication of such a dependence. The theoretical treatments of Bloch (1937), Halpern, Hamermesh & Johnson (1941), Ekstein (1949, 1950) and Halpern (1949) avoid touching on this problem. Also in the paper of Lax (1951, p. 289) this gap in the knowledge is made clear because he discusses only the two limiting cases of B normal and B tangential to the refractive boundary; he does not touch on the question of how the first passes to the second.

We therefore decided to measure this behaviour. We had at our disposal large iron (4 at. % Si) single crystals (15 mm diameter, 10 cm length) with well defined magnetic domain structures: disk-shaped domains all parallel to each other and normal to the crystal axis <110>. These walls are 90° Bloch walls with zigzag structure as shown in Fig. 1. The results of our measurements are given in Scharpf & Strothmann (1976) (see also the review paper of J. Scholten in this issue). The measurements were performed on a double-crystal spectrometer with silicon crystals, first used by Schneider & Shull (1971), with a resolution of 5°. Our result was that there was no dependence of the angle of deviation on the direction of magnetization on the two sides of the boundary, i.e. the above-cited statement of Bacon is wrong. But there remains the question of understanding these measurements in spite of the Halpern magnetic scattering vector, which is experimentally certain.

**Derivation of the magnetic index of refraction**

In the literature there can be found two different ways to derive an expression for the magnetic part of the index of refraction: (1) derivation by reduction to the magnetic scattering length of single atoms, analogous to the derivation of the index of refraction from nuclear scattering (Halpern, Hamermesh & Johnson, 1941; De Benedetti, 1964); (2) derivation with the dynamical theory of diffraction in the one-beam case (Ekstein, 1949). These derivations give the same result in the case of the mirror experiments of Hughes & Burgy (1951). If the magnetization \( \mathbf{\mu}_A \) is normal to the plane \( xy \) and to the incident wave vector, then \( Q \to 0 \) with \( k \to 0 \) (Fig. 3b), i.e. the component of the magnetization normal to the refractive boundary is ineffective for the determination of the index of refraction.

The results of this derivation can be expressed in the statement: For the determination of the index of refraction only the component of magnetization, which is reversed, in the refracting boundary is effective, e.g. \( B_z \) in Fig. 2. The component normal to the refracting boundary would play no role in the effective index of refraction and one should expect in the experiments a dependence of the angle of refraction on the component of magnetization parallel to the refracting boundary, which for Bloch walls can be varied with an applied field. Our experiments with Bloch walls cannot be brought into agreement with this statement, whereas the mirror experiments of Hughes & Burgy cannot disprove it.

The dynamical theory of diffraction of neutrons (Ekstein, 1949; Mendiretta & Blume, 1976) yields the refractive index, giving an expression for the wave vector if the transmitted wave is far from a Laue reflection. In this case the index of refraction includes both the magnetization component, which is reversed in the refracting boundary, and the two

\[
Q = \mathbf{\mu}_A \cdot \mathbf{k} - \mathbf{\mu}_A
\]

with \( \mathbf{\mu}_A \) = unit vector in the direction of magnetization, \( \mathbf{k} \) = unit vector in the direction of the scattering vector. The index of refraction is derived from the forward-scattering amplitude \( f(0) \) [whose magnetic term contains the factor \( Q(0) \)] by

\[
n - 1 = \frac{2\pi N}{k^2} f(0)
\]
other components of the magnetization. This total average magnetic induction, \( |\mathbf{B}| = (B_x^2 + B_y^2 + B_z^2)^{1/2} \), determines also the precession of the neutron spin in the interior of ferromagnetic materials, in spite of the fact that they possess a magnetic lattice. We show that in the following: The wave equation of the neutron in magnetic materials is

\[
(\nabla^2 + k_0^2)\psi - \frac{2m}{\hbar^2} \left\{ V(r) - \mu_n \sigma [\mathbf{H}(r) + 4\pi \mathbf{M}(r)] \right\} \psi = 0. \tag{3}
\]

\( \psi \) = spinor, \( \sigma \) = Pauli spin matrices, \( k_0 = \) modulus of the incident wave vector, \( \mu_n \) = magnetic moment of the neutron, \( m = \) mass of the neutron, \( \mathbf{H}, \mathbf{M}, V = \) field, magnetization and nuclear potential.

In a periodic lattice \( \mathbf{V, H, M} \) are periodic functions of \( r \) and can be given by Fourier series:

\[
\mathbf{V}(r) = \sum_v c_v \exp (2\pi i \mathbf{A}_v \cdot r),
\]

\[
\mathbf{M}(r) = \sum_v \mathbf{m}_v \exp (2\pi i \mathbf{A}_v \cdot r),
\]

\[
\mathbf{H}(r) = \sum_v \mathbf{h}_v \exp (2\pi i \mathbf{A}_v \cdot r),
\]

\[
\mathbf{m}_v = \frac{1}{\tau} \int_{\text{cell}} \mathbf{M}(r) \exp (-2\pi i \mathbf{A}_v \cdot r) dr,
\]

with \( \mathbf{A}_v = \) reciprocal-lattice vector, \( v = \) index of summation (triplet of integers), \( \tau = \) volume of the unit cell, which is also the volume of integration. Similar expressions to that for \( \mathbf{m}_v \) are obtained for \( c_v \) and \( \mathbf{h}_v \). Insertion of these Fourier series into the Maxwell equations gives

\[
\mathbf{A}_v \cdot (\mathbf{h}_v + 4\pi \mathbf{m}_v) = 0
\]

because \( \nabla \times \mathbf{B} = 0 \) and \( \mathbf{A}_v \times \mathbf{h}_v = 0 \) because \( \nabla \times \mathbf{H} = 0 \). For \( v \neq 0 \) one obtains

\[
\mathbf{h}_v = -4\pi \mathbf{A}_v (\mathbf{A}_v \cdot \mathbf{m}_v)/\mathbf{A}_v^2.
\]

\( \mathbf{A}_v = (0,0,0) \) yields \( v_0 = V_{A_v}, h_0 = H_{A_v}, m_0 = M_{A_v} \). Application of Bloch’s theorem yields for the wavefunction solving the Schrödinger equation (3) a spinor of the form

\[
\psi = \exp (i \mathbf{k} \cdot \mathbf{r}) \sum_v c_v \exp (2\pi i \mathbf{A}_v \cdot \mathbf{r})
\]

with \( c_v = \) constant spinors. We put

\[
(2m/\hbar^2) (\mathbf{V}(r) - \mu_n \sigma [\mathbf{H}(r) + 4\pi \mathbf{M}(r)]) = \sum_v \mathbf{w}_v \exp (2\pi i \mathbf{A}_v \cdot \mathbf{r}).
\]

i.e.

\[
\mathbf{w}_v = (2m/\hbar^2) [v_0 + 4\pi \mu_n \sigma (\mathbf{A}_v \cdot \mathbf{m}_v)/\mathbf{A}_v^2 - \mathbf{m}_v].
\]

Insertion of this Fourier series in the Schrödinger equation gives

\[
[k_0^2 - (\mathbf{k} + 2\pi \mathbf{A}_v)^2] c_v - \sum_v \mathbf{w}_v \cdot c_v = 0. \tag{3b}
\]

If the direction of \( \mathbf{k} \) is far from Laue reflection, then only \( c_v \) has a significant value and the Fourier series consist only of the first averaging expressions and we obtain the Schrödinger equation

\[
(\nabla^2 + k_0^2)\psi - \frac{2m}{\hbar^2} (V_{A_v} + \mu_n \sigma \mathbf{B}_{A_v}) \psi = 0. \tag{4}
\]

with

\[
\psi = c_0 \exp (i \mathbf{k} \cdot \mathbf{r}) \tag{4a}
\]

or

\[
(k_0^2 - k^2) c_0 - \omega_0 c_0 \approx 0.
\]

This is the so-called one-beam case. Equation (4) yields the refractive index

\[
n^2 = \frac{k^2}{k_0^2} = 1 - \frac{(\Delta k)^2}{k_0^2} \tag{5}
\]

with \( \mathbf{k} \) and \( \mathbf{k} \) wave vectors (\( \mathbf{k} \) of equation 4a) for spin parallel and antiparallel to \( \mathbf{B}_{A_v} \), and

\[
(\Delta k)^2 = (2m/\hbar^2) V_{A_v} = 4\pi N n_{coh} , \quad k_0^2 = (2m/\hbar^2) \mu_n |\mathbf{B}_{A_v}|.
\]

This result is the same as given above by Bacon’s equation (1).

But now we know additionally from (4) that this result is similar to that in electrodynamics where the description of the macroscopic behaviour in a medium by the Maxwell equations requires only an average magnetic induction \( \mathbf{B}_{A_v} \) (Jackson, 1965). The above derivation shows that the behaviour of neutrons in a magnetic material can be described by the same average magnetic induction \( \mathbf{B}_{A_v} \), and this is valid for all wavelengths and all directions except for those of Laue interfer-ences. One can see here very clearly how the dynamical theory yields an effective average magnetization, as we also observed in our spin-echo measurements with polarized neutrons traversing a homogeneously magnetized saturated ferromagnetic foil (Schärpf & Warnecke, 1976).

We conclude as a consequence of the above-quoted second method for the investigation of the magnetic refraction of neutrons with the direction of the wave vector far from a Laue reflection that it is possible to use regions of continuous homogeneous \( \mathbf{B} \) for the description of the interaction of the neutron with the magnetic induction and to introduce this in the Schrödinger equation (4) in the spin-dependent potential. Only for Laue reflections is the equivalent of the Halphen magnetic scattering vector effective (equations 3a,b).

Bloch walls as refractive boundaries are in the following considered as sharp transitions from a region with one direction of magnetization to a region with another direction of magnetization. The refractive behaviour is then a boundary-value problem.

**Refraction of neutrons at domain boundaries**

The geometry of the magnetization components on both sides of the Bloch wall is shown in Fig. 2 and is the geometry of a wall in the most general possible position without a divergence of the magnetization. For this reason, the wall has to lie symmetrically with respect to \( \mathbf{M}_{I} \) and \( \mathbf{M}_{II} \), the magnetization directions in the adjacent domains. But it is possible for the wall to be inclined at angle \( \psi \) to the direction normal to the plane of the magnetization directions \( \mathbf{M}_{I} \) and \( \mathbf{M}_{II} \). Fig. 2 shows the different components of \( \mathbf{B} \) (see also paper II). In domain I we have \( \mathbf{B} = (\mathbf{B}_x, \mathbf{B}_y, -\mathbf{B}_z) \) and in domain II \( \mathbf{B} = (\mathbf{B}_x, \mathbf{B}_y, +\mathbf{B}_z) \) with a jump at \( y = 0 \) from \( B_z = -B_z \). The two other components are the same in the two adjacent domains. With \( (2m/\hbar^2) \mu_n B_x = k_x^2 \) and \( (2m/\hbar^2) \mu_n B_z = k_z^2 \), we obtain the Schrödinger equation

\[
(\nabla^2 + k_0^2)\psi = \psi_1 \tag{4b}
\]

\[
\left( \begin{array}{c}
\psi_1 \\
\psi_2
\end{array} \right) = \left[ \begin{array}{c}
k_x \psi_1 \\
-k_x \psi_2
\end{array} \right] + \frac{2m}{\hbar^2} \left( \begin{array}{c}
-\psi_1 \\
\psi_2
\end{array} \right)
\]

\[
+ (k_y^2 + k_z^2) \left( \begin{array}{c}
-\psi_1 \\
\psi_2
\end{array} \right) = 0
\]

(minus sign in parentheses applies to domain II). As the potential is a function of \( y \) only, this equation has the solution
\[
\begin{align*}
  \begin{pmatrix}
    \psi_1 \\
    \psi_2
  \end{pmatrix} &= \exp \left[ i(k_2 x + k_2 z) \right]
  \begin{pmatrix}
    \phi_1(y) \\
    \phi_2(y)
  \end{pmatrix},
\end{align*}
\]

with

\[
\begin{align*}
  \begin{pmatrix}
    \phi_1 \\
    \phi_2
  \end{pmatrix} + \begin{pmatrix}
    (k_2^2 \pm k_2^2) & (k_2^2 - ik_2^2) \\
    (k_2^2 - ik_2^2) & (k_2^2 + ik_2^2)
  \end{pmatrix} \begin{pmatrix}
    \phi_1 \\
    \phi_2
  \end{pmatrix} &= 0. \quad (6)
\end{align*}
\]

If one solves this system of differential equations, by finding \( \phi_2 \) from the first equation and inserting this into the second equation, one obtains for \( \phi_1 \), a differential equation of fourth order with constant coefficients independent of the sign of \( k_2^2 \):

\[
\phi_1'' + 2k_2^2 \phi_1' + (k_2^4 - k_2^2 x^2 - k_2^2 y^2) \phi_1 = 0.
\]

With the characteristic equation

\[
\lambda^4 - 2k_2^2 \lambda^2 + (k_2^4 - k_2^2) = 0
\]

and

\[
k_x = \sqrt{k_2^2 - k_2^2}, \quad k_y = \sqrt{k_2^2 + k_2^2},
\]

one obtains the solution in domain I for \( y < 0 \):

\[
\begin{align*}
  \begin{pmatrix}
    \phi_1(y) \\
    \phi_2(y)
  \end{pmatrix} &= \begin{pmatrix}
    1 \\
    M
  \end{pmatrix} A_1 \exp (i k_x y) + \begin{pmatrix}
    1 \\
    M
  \end{pmatrix} A_2 \exp (-i k_x y) \\
  &+ \begin{pmatrix}
    1 \\
    -P
  \end{pmatrix} A_3 \exp (i k_y y) + \begin{pmatrix}
    1 \\
    -P
  \end{pmatrix} A_4 \exp (-i k_y y), \quad (8)
\end{align*}
\]

and in domain II with \( y > 0 \):

\[
\begin{align*}
  \begin{pmatrix}
    \phi_1(y) \\
    \phi_2(y)
  \end{pmatrix} &= \begin{pmatrix}
    1 \\
    P
  \end{pmatrix} \alpha_1 \exp (i k_x y) + \begin{pmatrix}
    1 \\
    P
  \end{pmatrix} \alpha_2 \exp (-i k_x y) \\
  &+ \begin{pmatrix}
    1 \\
    -M
  \end{pmatrix} \alpha_3 \exp (i k_y y) + \begin{pmatrix}
    1 \\
    -M
  \end{pmatrix} \alpha_4 \exp (-i k_y y)
\end{align*}
\]

with

\[
\begin{align*}
  M &= (k_2^2 - k_2^2)/(k_2^2 - ik_2^2) = \frac{ie^{-i\theta}(1 - \sin \theta_0) / \cos \theta_0}{\sin \theta_0^2} \\
  &= \frac{ie^{-i\theta} \tan [(90^\circ - \theta_0)/2]}{\sin \theta_0^2} \quad (9)
\end{align*}
\]

\[
\begin{align*}
  P &= (k_2^2 + k_2^2)/(k_2^2 - ik_2^2) = \frac{ie^{-i\theta}(1 + \sin \theta_0) / \cos \theta_0}{\sin \theta_0^2} \\
  &= \frac{ie^{-i\theta} \tan [(90^\circ + \theta_0)/2]}{\sin \theta_0^2}.
\end{align*}
\]

With the incident wave

\[
\begin{align*}
  \exp \left[ i(k_2 x + k_2 z) \right] \left[ \begin{pmatrix}
    1 \\
    M
  \end{pmatrix} A_1 \exp (i k_x y) \\
  + \begin{pmatrix}
    1 \\
    -P
  \end{pmatrix} A_3 \exp (i k_y y) \right], \quad (10)
\end{align*}
\]

the reflected wave

\[
\begin{align*}
  \exp \left[ i(k_2 x + k_2 z) \right] \left[ \begin{pmatrix}
    1 \\
    M
  \end{pmatrix} A_2 \exp (-i k_x y) \\
  + \begin{pmatrix}
    1 \\
    -P
  \end{pmatrix} A_4 \exp (-i k_y y) \right],
\end{align*}
\]

the transmitted wave

\[
\begin{align*}
  \exp \left[ i(k_2 x + k_2 z) \right] \left[ \begin{pmatrix}
    1 \\
    P
  \end{pmatrix} \alpha_1 \exp (i k_x y) + \begin{pmatrix}
    1 \\
    -M
  \end{pmatrix} \alpha_3 \exp (i k_y y) \right]
\end{align*}
\]

and the continuity conditions of the neutron current at the boundary \( y = 0 \), one obtains the linear system of equations:

\[
\begin{align*}
  A_1 + A_3 &= \alpha_1 + \alpha_3 - A_2 - A_4 \\
  A_1 M - A_3 P &= \alpha_1 - \alpha_3 M - A_2 M + A_4 P \\
  A_1 k_x - A_3 k_y &= \alpha_1 k_x - \alpha_3 k_y + A_2 k_y + A_4 k_y \\
  A_1 k_x M - A_3 k_y P &= \alpha_1 k_x P - \alpha_3 k_y M + A_2 k_y M - A_4 k_y P.
\end{align*}
\]
The solution of this system of equations can be given analytically. It yields the amplitudes of the reflected and transmitted waves and therewith the reflectivity and transmission of the direct and reflected beams, which are calculated by means of formulas analogous to equation (8) in paper II (see also discussion of it), with $E$ corresponding to $\alpha_1$ and $F$ corresponding to $\alpha_3$.

To discuss this solution, we consider first the incident wave with the spinor $(\psi)$. This spinor is

$$
\left( \frac{1}{M} \right) \frac{1}{\cos[(90°-\theta_0)/2]} \left( \cos[(90°-\theta_0)/2] \sin[(90°-\theta_0)/2] e^{-i\omega t} \right),
$$

where $\psi$ is the angle between the normal to the boundary and the plane of the magnetization directions. This spinor corresponds to a spin in the direction of magnetization in domain I but expressed in a coordinate system with the $z$ and $\chi$ directions as given in Fig. 2. The spinor $(\psi)$ is that of a neutron with spin antiparallel to the magnetization direction in domain II. The respective wave vectors correspond to this spin direction. The above spinor is normalized by a factor $A_1 = \cos[(90°-\theta_0)/2]$.

The incident wave of equation (10) consists of two parts, one with spin parallel and one with spin antiparallel to the magnetization. The part with $A_1(\psi)$ is the wave with spin parallel to magnetization.

Now the spin direction of a neutron traversing the infinitely thin wall remains fixed in space and only the wave vector is changed as a result of the new environment of the spin in domain II. Therefore the spin which was parallel to magnetization in domain I is now in domain II at an angle of $2\theta_0$ to magnetization. Correspondingly one has to resolve the spin into components parallel and antiparallel to the new direction of magnetization, and one obtains factors of $\cos^2 \theta_0$ in the part with spin parallel and $\sin^2 \theta_0$ in the part with spin antiparallel. This is also the result of the solution of the system of linear equations (11), including the reflected part of the wave.

These different parts also have different wave vectors. The part with $\cos^2 \theta_0$ has the same wave vector as before and therefore is not deflected. The part with $\sin^2 \theta_0$ has a spin antiparallel to the field and changes the $k_i$ component to $k_i$ and correspondingly the direction, i.e. it is deflected. The angle of deflection $\alpha$, can be calculated by means of

$$
\alpha = \arcsin \left[ \sqrt{\left( k_i \right)^2 + 2k_i B_i} \right] \left[ (2\pi/\lambda)^2 + k_i^2 \right] - \theta,
$$

with $\theta$ = grazing angle of incidence. It is noteworthy that $k_i^2$ does not contain just a component of $B$ but always the whole $B = (B_x^2 + B_y^2 + B_z^2)^{1/2}$ irrespective of the direction of $B$ on the two sides of the refractive boundary, i.e. even if the direction of magnetization is varied one has always the same angle of deflection; only the intensity of the refracted beam is changed and becomes zero if $\theta_0 \to 0$ in Fig. 1. Neither the angle of deflection, which can be determined from the wave vectors, nor the intensities of the reflected and transmitted beams depend on the angle $\psi$ (Fig. 1). Reflectivity and transmission resulting from the solution of equation (11) are given in Fig. 4(a-d). The deflection is given in Fig. 5. The calculations are made for neutrons with wavelength $\lambda=4\,\text{Å}$ and Bloch walls in iron. The calculated deflection for $\lambda=2.3\,\text{Å}$ agrees with that found in our measurements (Scharpf & Strothmann, 1976) and is really independent of $\theta_0$. The behaviour of the intensity is changed by the internal helical magnetic structure of the wall, as is further discussed in paper II.

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References


